Table: Names

The "Names" table has the names and description of the molecules.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
Species		xs:string	Chemical Formula for molecule
Name		xs:string	Name of molecule (not systematic)
heavies		xs:integer	How many heavy (not H or He) atoms.
MaxAtNo		xs:integer	Maximum atomic number in molecule. For H2SO4 it is S, so 16.
atoms		xs:integer	Number of atoms in molecule.
sumatno		xs:integer	Sum of atomic numbers. For H2SO4 it would be 1+1+16+8+8+8+8 = 50
maxcolno		xs:integer	Maximum periodic table column number. For H2SO4 is would be S or O = 6
sumcolno		xs:integer	Sum of column numbers. For H2SO4 it is 1+1+6+6+6+6+6 = 32
ssqcolno		xs:integer	Sum of the squares of the column numbers. For H2SO4 it is 1+1+36+(36)*4 = 182
omit		xs:byte	Leave this out of web pages

Table: Formula

The "Formula" table has the explicit list of atoms in the molecule.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
formula		xs:string	Name of molecule (not systematic)
filename		xs:string	The name used on the directory that contains this molecule.
H		xs:integer	How many H atoms
He		xs:integer	How many He atoms.
Li		xs:integer	How many Li atoms.
Be		xs:integer	How many Be atoms.
B		xs:integer	How many B atoms.
C		xs:integer	How many C atoms.
N		xs:integer	How many N atoms.
O		xs:integer	How many O atoms.
F		xs:integer	How many F atoms.
Ne		xs:integer	How many Ne atoms.
Na		xs:integer	How many Na atoms.
Mg		xs:integer	How many Mg atoms.
Al		xs:integer	How many Al atoms.
Si		xs:integer	How many Si atoms.
P		xs:integer	How many P atoms.
S		xs:integer	How many S atoms.
Cl		xs:integer	How many Cl atoms.
Ar		xs:integer	How many Ar atoms.
K		xs:integer	How many K atoms.
Ca		xs:integer	How many Ca atoms.
Sc		xs:integer	How many Sc atoms.
Ti		xs:integer	How many Ti atoms.
V		xs:integer	How many V atoms.
Cr		xs:integer	How many Cr atoms.

Field	Unit	Type	Description
Mn		xs:integer	How many Mn atoms.
Fe		xs:integer	How many Fe atoms.
Co		xs:integer	How many Co atoms.
Ni		xs:integer	How many Ni atoms.
Cu		xs:integer	How many Cu atoms.
Zn		xs:integer	How many Zn atoms.
Ga		xs:integer	How many Ga atoms.
Ge		xs:integer	How many Ge atoms.
As		xs:integer	How many As atoms.
Se		xs:integer	How many Se atoms.
Br		xs:integer	How many Br atoms.
Kr		xs:integer	How many Kr atoms.
Rb		xs:integer	How many Rb atoms.
Sr		xs:integer	How many Sr atoms.
Y		xs:integer	How many Y atoms.
Zr		xs:integer	How many Zr atoms.
Nb		xs:integer	How many Nb atoms.
Mo		xs:integer	How many Mo atoms.
Jg		xs:integer	How many Jg atoms.
Ru		xs:integer	How many Ru atoms.
Rh		xs:integer	How many Rh atoms.
Pd		xs:integer	How many Pd atoms.
Ag		xs:integer	How many Ag atoms.
Cd		xs:integer	How many Cd atoms.
In		xs:integer	How many In atoms.
Sn		xs:integer	How many Sn atoms.
Sb		xs:integer	How many Sb atoms.
Te		xs:integer	How many Te atoms.
I		xs:integer	How many I atoms.
D		xs:integer	How many D atoms.

Field	Unit	Type	Description
X		xs:integer	How many dummy atoms used for z-matrix.
mass	amu	xs:float	Mass in amu.
symno		xs:integer	Symmetry number
polyatomic			atom, linear or poly
nval		xs:integer	Number of valence electrons in molecule. H2SO4 has 1+1+6+6+6+6+6 = 32
omit		xs:byte	Leave this out of web pages
Hill		xs:string	Hill Formula order of atoms in formula (C, then H, then alphabetical)
vibs		xs:integer	Number of vibrations in molecule.

Table: Inchis

The InChIs table contains the InChI String - a unique molecular identifier.
For more information see: http://www.inchi-trust.org/technical-faq/

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
standard		xs:integer	O is standard InChI, 1 is extended InChI/
inchi		xs:string	InChI string.
inchikey		xs:string	InChI hashed string.
smiles		xs:string	SMILES string.

Table: configs

The configs table has a description of the conformation and electronic state

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
statedescription			Symmetry label, such as 1A1 (for singlet A1) or 2PI.
confdescription			conformation label, sometimes the pointgroup (C2V) and sometimes words
filename		xs:string	Name used on directory that contains this molecule.

Table: bondlist

The table Bondlist has a list of which atoms are connected in a molecule.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
atomnumber		xs:int	Arbitrary number given to atom within a specific molecule.
atom1		xs:integer	atom connected to - specific atom -
atom2		xs:integer	atom connected to - specific above atom -
atom3		xs:integer	atom connected to - specific above atom -
atom4		xs:integer	atom connected to - specific above atom -
atom5		xs:integer	atom connected to - specific above atom -
atom6		xs:integer	atom connected to - specific above atom -

Table: Othernames

The table Othernames has synonyms for the molecule.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
unikey		xs:integer	Integer key for this table
othername			synonym for molecule
expose			This checkbox determines whether a molecule's synonym is shown on the web page. It is possible that mispellings are captured in the database, but not exposed on the website.
iupac			Is this the IUPAC standard name?

Table: references

The table References contains the bibliographic reference for the data

Field	Unit	Type	Description
squib		xs:string	About 16 charcaters describing the reference.
category		xs:string	Used to describe the general papers on geometry or vibrations, etc.
reference		xs:string	Reference text.
doi		xs:string	DOI for reference.
journal		xs:string	Abbreviated citation from Cross-Ref.

Table: ExpCartesians

The table ExpCartesians contains the cartesian coordinates (x,y,z) for a molecule.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
atomnumber		xs:int	Arbitrary number given to atom within a specific molecule.
atomtype		xs:integer	Atomic number of a given atom.
x	Angstrom	xs:float	X coordinate
y	Angstrom	xs:float	Y coordinate.
z	Angstrom	xs:float	Z coordinate.
squib		xs:string	About 16 charcaters describing the reference.

Table: ExpCoords

The table ExpCoords contains the bond lengths and angles and dihedrals.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
coordinate		xs:int	Sequential number for coordinate in molecule, 1 per unique coordinate. E.g. H2O has one unique bond length and one angle, also used as a foreign key.
bond_index		xs:integer	Field no longer used.
specific_description		xs:string	Description with multiple bonds indicated. Starts with r for bond; a for angle; d for dihedral. rC=O, aHC=O. = is double bond, # is triple bond.
description		xs:float	Description without bonds. Eg. rCO, aHCO
value	Angstrom or degree	xs:float	Bond length (Angstrom), bond angles (degrees), dihedrals (degrees)
value_unc	Angstrom or degree	xs:string	Uncertainty measured Angstrom or degrees.
squib		xs:string	About 16 charcaters describing the reference.
comment		xs:string	Help to specify coordinate.

Table: ExpCoordAtoms

The table ExpCoordsAtoms contains which atoms are involved in a coordinate. 2 for bonds, 3 for angles, 4 for dihedral

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
coordinate		xs:int	Sequential number for coordinate in molecule, 1 per unique coordinate. E.g. H2O has one unique bond length and one angle, also used as a foreign key.
udex		xs:int	For when one corrdinate describes more than pair (or triple) of atoms. Like the two O-H bonds in H2O.
atom1ECA			Atom1 in bond or angle
atom2ECA			Atom2 in bond or angle
atom3ECA			Atom3 in bond or angle
atom4ECA			Atom4 in bond or angle

Table: ExpEnthalpy

The table ExpEnthalpy contains the enthalpy of formation at 298K and 0K.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
Hfg	kJ/mol	xs:string	Enthalpy of formation of the molecule at 298.15K.
Hfg_unc	kJ/mol		Uncertainty in Enthalpy of Formation
Hfg_0K	kJ/mol		Enthalpy of formation of the molecule at 0K.
squib		xs:string	About 16 charcaters describing the reference.
comment			Comment on Enthalpy.

Table: ExpRot

The table ExpRot contains the 1 or three rotational constants.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
symno		xs:integer	Symmetry number
polyatomic			atom, linear or poly
a	cm^{-1}		A rotational Constant. Null for linear molecules
b	cm^{-1}		B rotational Constant. Must be non-null.
c	cm^{-1}		C rotational Constant. May be used or null for linear molecules.
squib		xs:string	About 16 charcaters describing the reference.
comment			Comment

Table: ExpVibrations

The table ExpVibrations contains the vibrational frequencies (and maybe Intensities) of the molecule.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
modeindex		xs:int	Unique key for each vibrational frequency
modenumber			Traditional number with degenerate groups of vibrations having the same number.
unique			Bit used to exclude repeat listings of degenerate modes. Frequency with th elowest modeindex is marked as unique.
symmetry			Symmetry of vibrational mode. A1, B2, Pi, Sg, E1. These are formatted by the web pages
frequency	cm^{-1}		Vibrational frequency
squib		xs:string	About 16 charcaters describing the reference.
comment			Comment
intensity	km/mol		Intensity of vibrational mode
intensityunc			Uncertainty of Intensity of vibrational mode
intsquib			Reference for intensity.

Table: ExpEntropy

The table ExpEntropy contains the Entropy (S) of moleculs at 298.15 K.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
entropy	J/mol K		Entropy of molecule at 298.15 K.
entropy_unc	J/mol K		Uncertainty of Entropy of molecule at 298.15 K.
squib		xs:string	About 16 charcaters describing the reference.
comment			Comment

Table: ExpHH

The table ExpHH contains the Integrated Heat Capacity of molecules.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
HH	kJ/mol		Integrated Heat Capacity
HH_unc	kJ/mol		Uncertainty of Integrated Heat Capacity.
squib		xs:string	About 16 charcaters describing the reference.
comment			Comment

Table: ExpDipole

The table ExpDipole contains the electric dipole moment.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
dipx	D		x component of the dipole moment, sometimes a component as noted in comment
dipy	D		Z component of the dipole moment, sometimes b component
dipz	D		Z component of the dipole moment, sometimes c component
diptot			Total dipole moment.
squib		xs:string	About 16 charcaters describing the reference.
comment		xs:string	Comment

Table: ExpIonEnergies

The table "ExpIonEnergies" contains the adiabatic and vertical ionization energies.

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
IE	eV		Ionization Energy (Adiabatic)
IE_unc	eV		Uncertainty of Ionization Energy
IE_vert	eV		Vertical Ionization Energy
IE_vert_unc	eV		Uncertainty of Vertical Ionization Energy
squib		xs:string	About 16 charcaters describing the reference.
comment		xs:string	Comment

Table: ExpPolarizability

The table ExpPolarizability contains experimental polarizabilities

Field	Unit	Type	Description
casno		xs:int	Chemical Abstract Number. Some are not consistant with Chemical Abstract Service.
charge		xs:int	Charge on molecule.
state		xs:int	Number for the electronic state. 1 is ground state, 2 is next higher exctited state.
config		xs:int	Number for conformation. 1 is usually most symmetric, 2 is less so, etc,
alpha	Angstrom cubed		total anisotropic polarizability.
unc	Angstrom cubed		Uncertainty in total anisotropic polarizability.
xx	Angstrom cubed		xx component of polarizability
xy	Angstrom cubed		xy component of polarizability.
yy	Angstrom cubed		yy component of polarizability.
xz	Angstrom cubed		xz component of polarizability.
yz	Angstrom cubed		yz component of polarizability.
zz	Angstrom cubed		zz component of polarizability.
squib		xs:string	About 16 charcaters describing the reference.
comment		xs:string	Comment